XXIX Symposium on Bioinformatics and Computer-Aided Drug Discovery

DEVELOPMENT OF A STANDARDIZED APPROACH FOR TRANSFER LEARNING WITH QSAR MODELS

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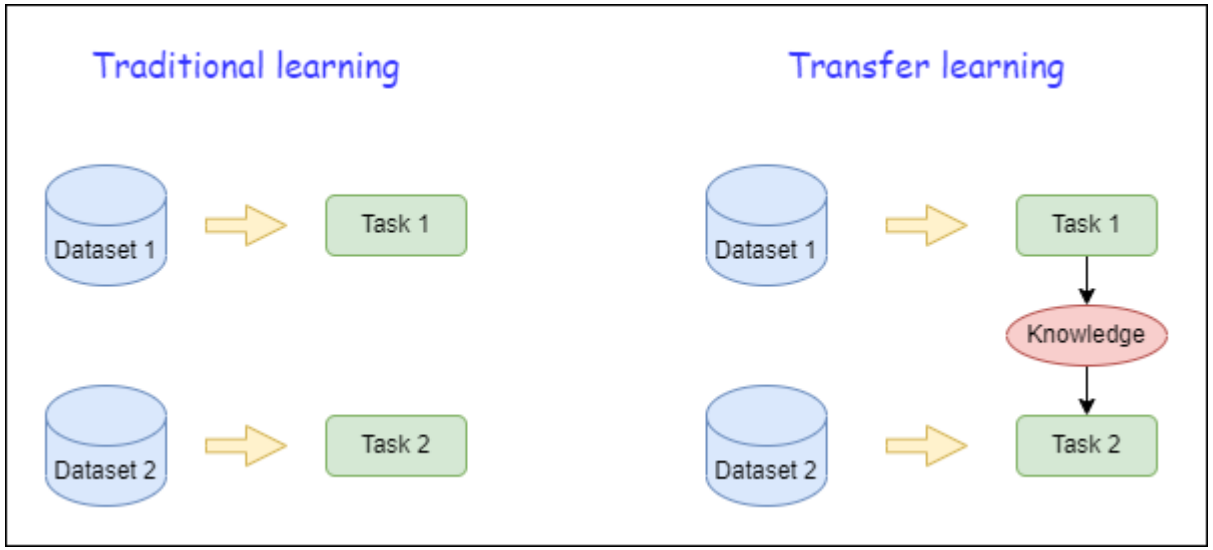
INTRODUCTION

- What is transfer learning?



INTRODUCTION

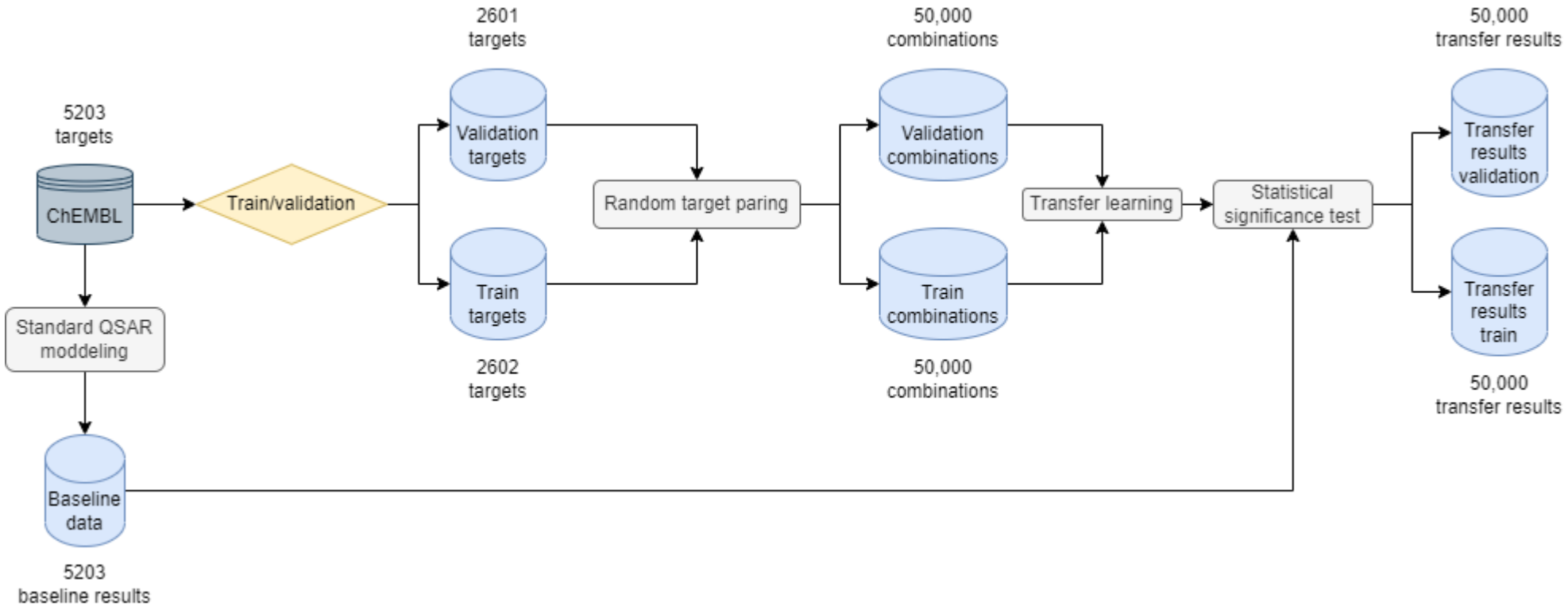
- How are we going to transfer information from the source task to the target task?
- Which targets should we use as source tasks for a particular target task of interest?

OBJECTIVES

- Creating a model capable of predicting the successfulness of a transfer between two datasets

- Creating a standardized transfer learning protocol capable of being implemented in an algorithmic manner

MATERIALS AND METHODS



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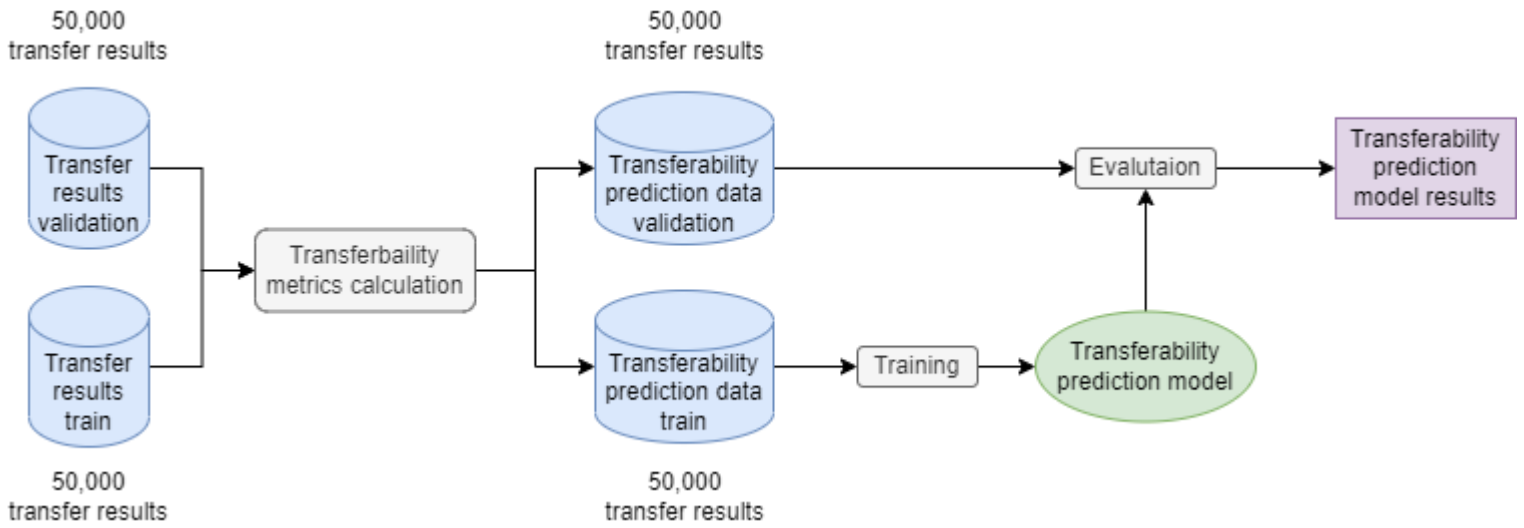

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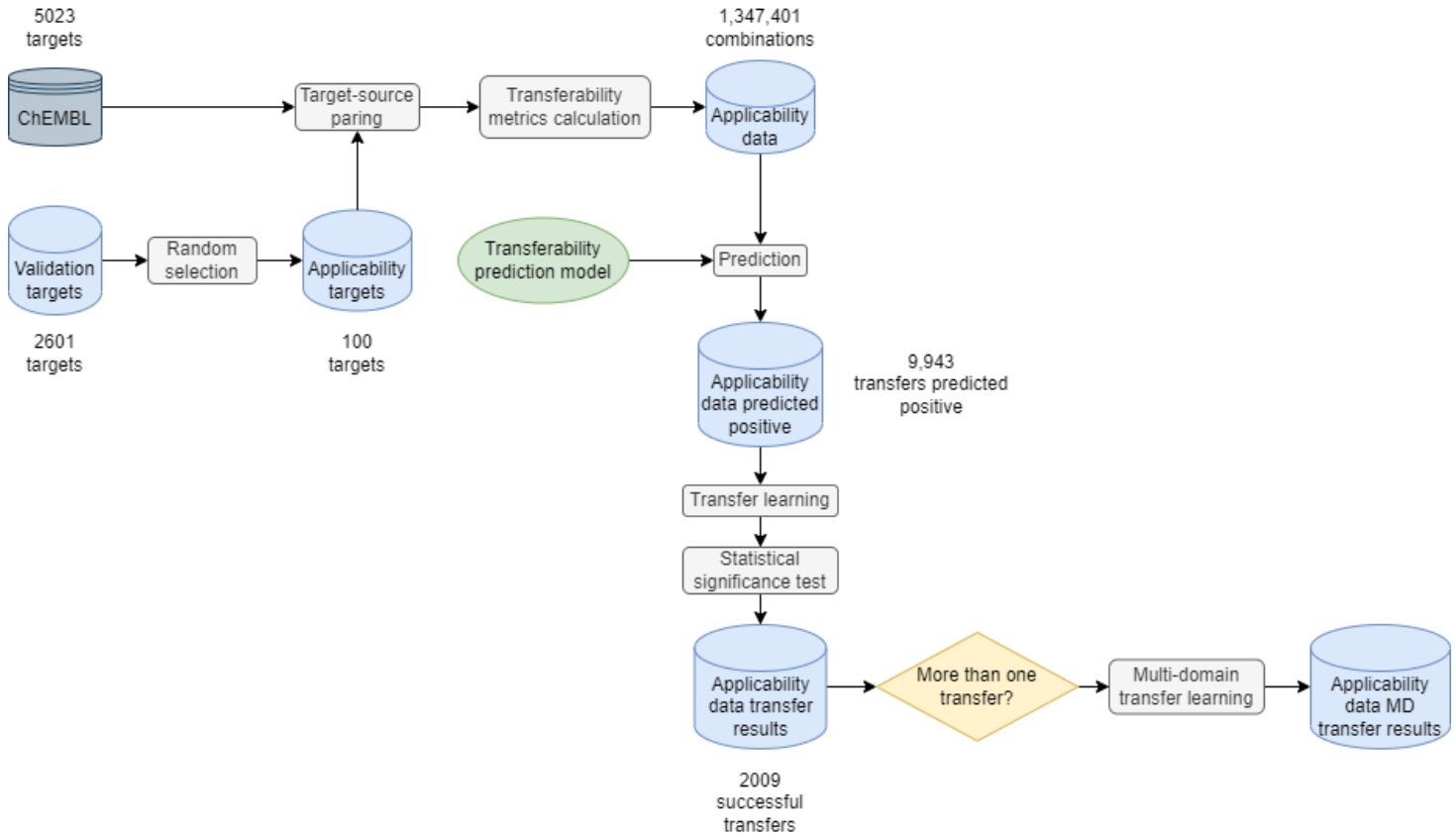
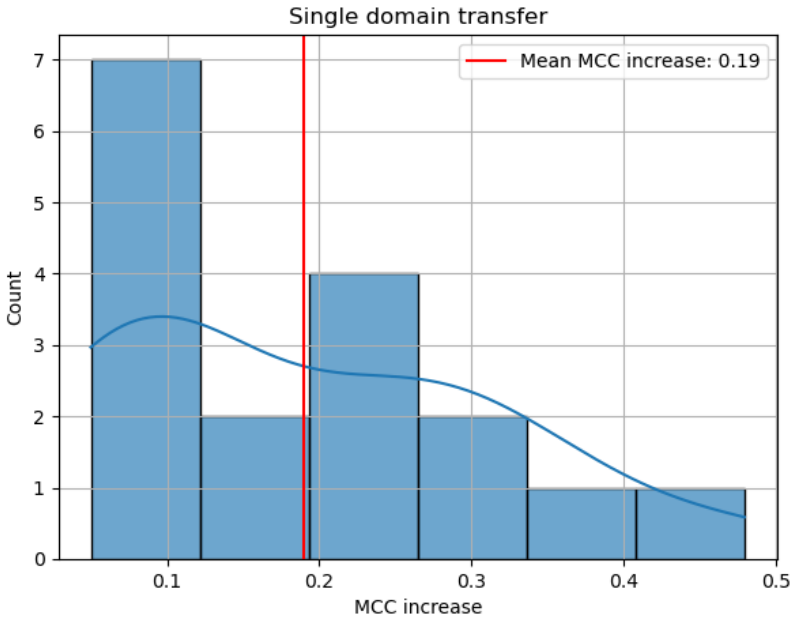
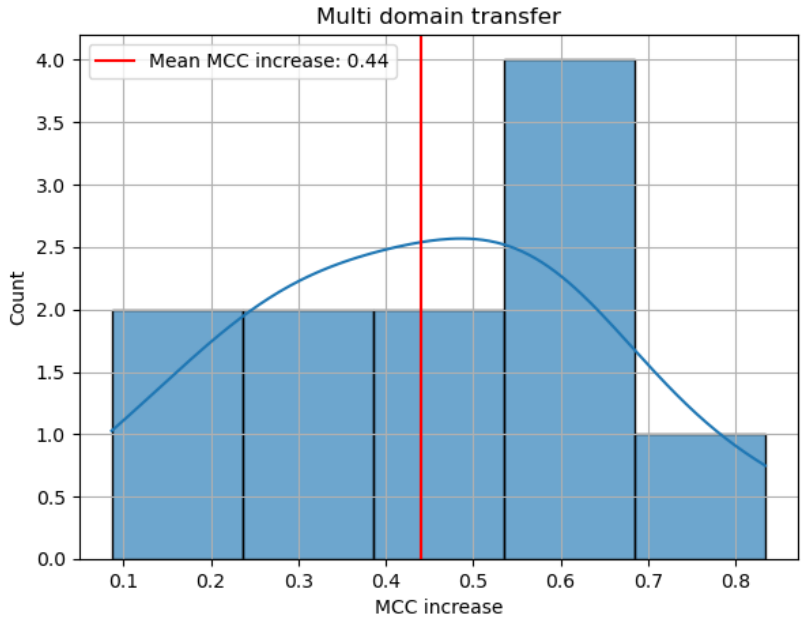


RESULTS AND DISCUSSION

- Successful transfers are very rare, with a probability of occurence of 0.126%
- The transferability prediction model achivied a precision of 17%, which representes a 127 times increase when compared to random chance
- The transferability prediction model was capable of identifying the majority of the successful transfers achieving a sensitivity of 92%
- Out of the 100 targets selected in the applicability subset 17 had at least one significant transfer identified
- Cell-lines are highly transferable amongst each other

RESULTS AND DISCUSSION





CONCLUSION

- Successful transfers are very rare
- Transfer learning as limited applicability even when source datasets are avaliable
- Finding a successful transfer in a naive manner is much less efficient than using a transferability prediction model
- Transfer learning can provide considerable performance increases on QSAR models

THANK YOU!

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